Coupling Atomic and Continuum Scales: Balance Laws and Basis Sets

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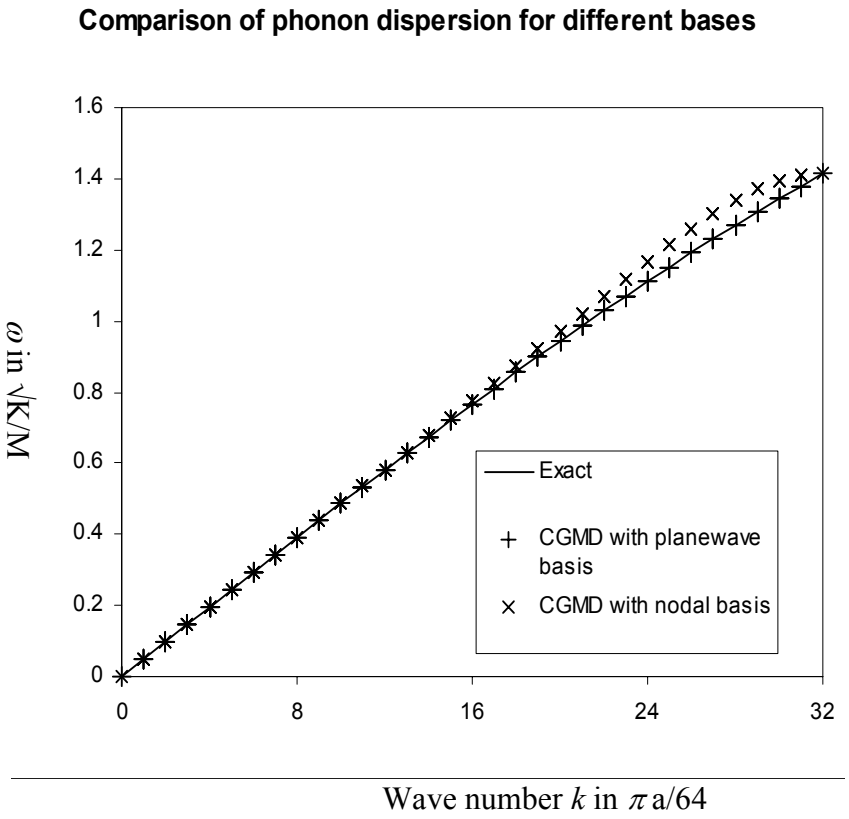
Research:

Many problems in mechanics include both atomistic and continuum phenomena. Strategies to address these problems typically assume specific atomic and continuum methods, typically coupled with *kinematic or least-squares fit constraints* that may not satisfy balance of momentum and energy. Such 'ad hoc' strategies tend to include correction terms that work for quasistatics but break down for dynamics. We are investigating how to couple reliably through a balance law formulation that is not based on specific 'a priori' choices of atomic and continuum methods.

We have shown, for example, for one coupling method, i.e. *coarse-grained molecular dynamics* (CGMD, Rudd and Broughton, PRB 58, R5893 (1998)), allowing greater freedom in the continuum basis provides greater accuracy [see figure]. We anticipate that use of the balance-law coupling will have similar advantages, but avoid the pathological problems in CGMD.

Work performed by graduate students B. Kraczek (Physics) and C. Xia (Theoretical and Applied Mechanics).



1-D phonon dispersion: Comparison of CGMD solutions for phonon dispersion employing plane-wave and nodal polynomial bases. While CGMD with a nodal basis reduces error relative to standard finite element methods, choosing the correct *continuum basis* shows the problem can be solved to arbitrary accuracy.